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Robust Integration Schemes for Generalized Viscoplasticity With Internal-State Variables

Part II Algorithmic Developments and Implementation

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ABSTRACT

This two-part report is concerned with the development of a general framework for the implicit time-stepping integrators for the flow and evolution equations in generalized viscoplastic models. The primary goal is to present a complete theoretical formulation, and to address in detail the algorithmic and numerical analysis aspects involved in its finite element implementation, as well as to critically assess the numerical performance of the developed schemes in a comprehensive set of test cases. On the theoretical side, the general framework is developed on the basis of the unconditionally-stable, backward-Euler difference scheme as a starting point. Its mathematical structure is of sufficient generality to allow a unified treatment of different classes of viscoplastic models with internal variables. In particular, two specific models of this type, which are representatives of the present state-of-art in metal viscoplasticity, are considered in applications reported here; i.e., fully associative (GVIPS) and non-associative (NAV) models. The matrix forms developed for both these models are directly applicable for both initially isotropic and anisotropic materials, in general (three-dimensional) situations as well as subspace applications (i.e., plane stress/strain, axisymmetric, generalized plane stress in shells). On the computational side, issues related to efficiency and robustness are emphasized in developing the (local) iterative algorithm. In particular, closed-form expressions for residual vectors and (consistent) material tangent stiffness arrays are given explicitly for both GVIPS and NAV models, with their maximum sizes "optimized" to depend only on the number of independent stress components (but independent of the number of viscoplastic internal state parameters). Significant robustness of the local iterative solution is provided by complementing the basic Newton-Raphson scheme with a line-search strategy for convergence. In the present second part of the report, we focus on the specific details of the numerical schemes, and associated computer algorithms, for the finite-element implementation of GVIPS and NAV models.

Robust Integration Schemes for Generalized Viscoplasticity with Internal-State Variables; Part II Algorithmic Developments and Implementation

1. Introduction

The scope of the work in this report focuses on the implementation and algorithmic developments of two classes of viscoplastic models: GVIPS (fully-associative) and NAV (nonassociative) based on the theory discussed in Part I [41] of the report. In the computer implementation of a viscoplastic model, the computational algorithm is the key ingredient. Over the past years considerable research effort has been devoted to the development of computational algorithms [1-9, 12, 16-50]. As discussed in Part I [41] of the report, initially, simple explicit integration schemes were predominate in finite element applications because of their ease in implementation, and because they do not require evaluating and inverting a Jacobian matrix. However, explicit integrators may not be efficient. That is, too many iteration steps may be required and convergence stability can not be guaranteed [32, 36, 50]. As a result, several alternative approaches have been used, for example, Gear's multi-step method [14] and Walker's asymptotic method [47]. Note that every integration scheme has its own particular application domain and is very problem dependent. For practical problems, it is desirable to use an unconditionally stable integration scheme in order to obtain an accurate solution. Recent work has clearly emphasized the use of implicit integration methods [4-6, 12, 16, 19-20, 23-24, 29, 31, 35, 37-38, 40, 43-44, 46, 48-49] in view of their superior stability and convergence properties [18, 34]. From the standpoint of practical applications, the one-step, fully implicit, backward Euler scheme is presently one of the most widely used integrators [6, 16, 18-20, 23, 31, 34, 35, 38, 39, 43, 44, 48, 49]. For the computationally intensive viscoplastic applications, found in typical finite element analysis, implicit backward Euler

integration methods have become the proven standard for the numerical integration of the viscoplastic rate equations [15, 40]. Details on the implementation of both classes of viscoplastic models (NAV, GVIPS) will be discussed in this report.

Based on the *fully implicit*, backward Euler scheme, the corresponding *algorithmic* (consistent) tangent stiffness arrays are derived from the integration rule, which are important for finite element solutions using (global) Newton-Raphson iterative methods. Explicit, closed-form, expressions for state variables and consistent tangent stiffness matrixes are given for the general three-dimensional (3D) situations, as well as for their *direct* modifications for the efficient treatment of two-dimensional (2D) or *subspace* applications; i.e., "generalized" plane stress states in shells. For these latter 2D problems, this simply amounts to "appropriate" reduction in the dimensions of the arrays involved, which is known to be more effective than alternative implementations [e.g., 12, 49], in which indirect (iterative) methods are used to handle the zero-stress constraints.

Beginning with the second section, and for the remainder of the report, *all* equations and expressions are shown using concise *matrix* notations for the integrated stress and internal stress fields. The contracted (Voigt) representations in *vector* forms for the components of the corresponding *symmetric, second-order*, tensor are utilized and the appropriate dimensions for the space of these vectors are defined explicitly; i.e., a six-dimensional space for 3D continuum problems, etc. With a slight abuse in notations to indicate the vector-matrix representations, matrices are defined by under-curved symbols, and vectors by underlined symbols, and $\otimes$ is used to indicate the tensor product of two vectors. Considering vectors a, b and c of dimension (6x1) in the 3D case, we define the matrix $(a \otimes b)c=(b \bullet c)a$, where "$\bullet$" signifies the inner (scalar) product of two vectors, and ":" for a double contraction C:D (or $C_{ijkl}\, D_{kl}$) and for tensor product $u \otimes w$ (or $u_i\, w_j$). Note that $\underline{\varepsilon^p}$ indicates the inelastic strain.

Section 2 deals with the implementation of the GVIPS class of models, as described in Part I [41], and similarly section 3 explains the implementation of the NAV class models. Although

the implicit backward Euler integration scheme is stable, for highly-nonlinear viscoplastic models, convergence may be difficult for certain problems. As a result, line search, a numerical technique based on optimization theory, is utilized to guarantee convergence and improve efficiency of the integrator. Details of the line search method are discussed in section 4.

1.1 General Form of Newton Iterative Scheme

The backward-Euler scheme is based on the equation

$$\underline{\Sigma}_{n+1} = \underline{\Sigma}_n + \Delta\underline{\Sigma}_{n+1} \tag{1.1}$$

where $\underline{\Sigma}_n$ is state variables, and $\Delta\underline{\Sigma}_{n+1}$ is the increment of the state variables. n is the step counter. For the GVIPS models,

$$\underline{\Sigma}_n = \begin{pmatrix} \underline{\sigma}_n \\ \underline{\alpha}_n \end{pmatrix} \tag{1.2}$$

for the NAV models,

$$\underline{\Sigma}_n = \begin{pmatrix} \underline{\sigma}_n \\ \underline{\alpha_s}_n \\ \underline{\alpha_l}_n \\ D_n \end{pmatrix} \tag{1.3}$$

the expression for the state variables' increment is

$$\Delta\underline{\Sigma}_{n+1} = \left(\underset{\sim}{K}_{\Sigma}\right)^{-1} \underline{R}_{n+1} \tag{1.4}$$

where $\underset{\sim}{K}_{\Sigma}$ is iterative Jacobi matrix of state variables, $\underline{R}_{n+1}$ is the residual function of state variables. The specific forms of $\underset{\sim}{K}_{\Sigma}$ and $\underline{R}_{n+1}$ for GVIPS and NAV are given subsequently.

2. Implicit Integration Scheme: GVIPS Class

The details of the integration algorithm, using the fully-implicit Euler method, for the specific GVIPS model (described in Part I [41]) are given below. For convenience in implementation, all equations of this GVIPS model are written in a vector-matrix format. This model serves as an example for discussing the implicit integration scheme.

2.1. The General Form

The hyperelastic response of the model is assumed to be *linear*; i.e., the Cauchy (true) stress components σ are given by

$$\underline{\sigma} = \underset{\sim}{C}^{e}\left(\underline{\varepsilon} - \underline{\varepsilon}^{p}\right) \quad ; \quad \underline{\varepsilon} = \underline{\varepsilon}^{e} + \underline{\varepsilon}^{p} \tag{2.1}$$

The governing equations for GVIPS are:

$$\dot{\underline{\varepsilon}}^{p} = f(F)\underline{\Gamma} \quad ; \quad \underline{\Gamma} = \underset{\sim}{M}(\underline{\sigma} - \underline{\alpha}) \tag{2.2}$$

$$\dot{\underline{\alpha}} = \underset{\sim}{L}^{-1}\left[\dot{\underline{\varepsilon}}^{p} - \frac{\gamma}{h}(G)\underline{\pi}\right] \quad ; \quad \underline{\pi} = \underset{\sim}{M}\,\underline{\alpha} \tag{2.3}$$

where,

$$F = \frac{1}{2}(\underline{\sigma} - \underline{\alpha})\underset{\sim}{M}(\underline{\sigma} - \underline{\alpha}) / K_t^2 - 1 \tag{2.4a}$$

$$G = \frac{1}{2}\underline{\alpha}\,\underset{\sim}{M}\,\underline{\alpha} / K_t^2 \tag{2.4b}$$

in which the symmetric matrix $\underset{\sim}{M}$ is a function of the fiber direction and is rewritten as

$$\underset{\sim}{M} = \underset{\sim}{P} - \xi \underset{\sim}{Q} - \frac{1}{2}\zeta \underset{\sim}{R} \tag{2.5}$$

where $\underset{\sim}{P}$, $\underset{\sim}{Q}$, and $\underset{\sim}{R}$ are symmetric matrices as defined in Part I [41].

In eq. (2.3),

$$\underset{\sim}{L}^{-1} = h\left[\underset{\sim}{Z}^{m} + \frac{h'}{h(1+2\beta)}\underline{\alpha} \otimes \underline{\alpha}\right] \tag{2.6a}$$

In the above equations, f, h, and γ are material functions which are defined as follows,

$$f(F) = F^{n} / \left(2\mu K_t \sqrt{F+1}\right) \tag{2.6b}$$

$$h = H / G^{\beta} \quad ; \quad \gamma = RG^{m-\beta} / \left(K_t \sqrt{G}\right) \tag{2.6c}$$

with, n, m, μ, K_t, H, β, and R denoting material dependent constants. In addition, the "generalized inverse" of $\underset{\sim}{M}$ is defined as follows:

$$\underset{\sim}{Z}^{m} = \underset{\sim}{M}^{-1} \tag{2.7a}$$

with $\underset{\sim}{M}$ directly evaluated from eq. (2.5) for the case of plane-stress continuum (with dimension 3×3) and generalized plane stress in shells (with dimension 5×5), but for the *three-dimensional* case, $\underset{\sim}{P}$ (6×6 dimension) in eq. (2.5) needs to be replaced by

$$\underset{\sim}{P} = diag[1,1,1,2,2,2] \tag{2.7b}$$

with its appropriate direct reduction to (4 × 4) for the axisymmetric/plane-strain continuum problems, that is,

$$\underset{\sim}{P} = diag[1,1,1,2] \tag{2.7c}$$

In the above, diag [·] indicates a diagonal matrix with entries [·].

The basic problem considered here is as follows. Consider a typical time step $t_n \rightarrow t_{n+1}$, where the state variables at t_n are known; i.e., $\{\sigma_n, \alpha_n, \varepsilon_n^p\}$. Let $\Delta t = t_{n+1} - t_n$, and $\Delta\varepsilon = \Delta t\dot{\varepsilon} = \varepsilon_{n+1} - \varepsilon_n$ be the *given* increment in the total strain field. Based upon the quantities at t_n, it is required to update to time t_{n+1} the above fields $\{\sigma_{n+1}, \alpha_{n+1}, \varepsilon_{n+1}^p\}$ in a manner consistent with the governing equations; i.e., eqs. (2.2, 2.3) for $\dot{\underline{\varepsilon}}^p$ and $\dot{\underline{\alpha}}$, and the *rate* form of eq. (2.1) for $\dot{\sigma}$, i.e.,

$$\dot{\underline{\sigma}} = \underset{\sim}{C}^e\left(\dot{\underline{\varepsilon}} - \dot{\underline{\varepsilon}}^p\right) \qquad ; \quad \dot{\underline{\varepsilon}} = \dot{\underline{\varepsilon}}^e + \dot{\underline{\varepsilon}}^p \tag{2.8a}$$

the matrix form of eq. (2.3) may be written as,

$$\dot{\underline{\alpha}} = \underset{\sim}{L}^{-1}\left[f\underline{\Gamma} - \frac{\gamma}{h}\underline{\pi}\right] \tag{2.8b}$$

Using the implicit Euler scheme, these update formulas are given as

$$\underline{\sigma}_{n+1} = \underline{\sigma}_n + \underset{\sim}{C}^e\left[\Delta\underline{\varepsilon} - \Delta t f\underline{\Gamma}_{n+1}\right] \tag{2.9a}$$

$$\underline{\alpha}_{n+1} = \underline{\alpha}_n + \Delta t\,\underset{\sim}{L}^{-1}\left[f\underline{\Gamma}_{n+1} - \frac{\gamma}{h}\underline{\pi}_{n+1}\right] \tag{2.9b}$$

where

$$f = f\left(\sigma_{n+1},\ \alpha_{n+1}\right) \quad ; \quad h = h\left(\alpha_{n+1}\right) \quad ; \quad \gamma = \gamma\left(\alpha_{n+1}\right) \tag{2.10}$$

2.2 Iterative Solution for Updated Fields

To determine the updated values for the state variables ($\underline{\sigma}_{n+1}$, $\underline{\alpha}_{n+1}$), a *local* iterative solution (i.e., distinct from global equilibrium iterations in finite elements) is needed based on the system of equations in Eqs. (2.1 and 2.3). To this end, we apply the Newton-Raphson scheme by first forming the *residual* vectors

$$\underline{R}_\sigma = \underline{\sigma}_{n+1} - \left[\underline{\sigma}_n + \underset{\sim}{C}^e\left(\underline{\Delta\varepsilon} - \Delta t f \underline{\Gamma}\right)\right] \tag{2.11a}$$

$$\underline{R}_\alpha = \underline{\alpha}_{n+1} - \underline{\alpha}_n - \Delta t \underset{\sim}{L}^{-1}\left[f\underline{\Gamma} - \frac{\gamma}{h}\underline{\pi}\right] \tag{2.11b}$$

A truncated Taylor's expansion for the $\underline{R}$ vectors about the last updated state then yields, for a typical iteration $k \rightarrow k+1$:

$$\underline{\sigma}_{n+1}^{k+1} = \underline{\sigma}_{n+1}^{k} + \Delta\underline{\sigma}_{n+1}^{k} \tag{2.12a}$$

$$\underline{\alpha}_{n+1}^{k+1} = \underline{\alpha}_{n+1}^{k} + \Delta\underline{\alpha}_{n+1}^{k} \tag{2.12b}$$

where

$$\Delta\underline{\sigma}_{n+1}^{k} = -\underset{\sim}{J}^{-1}\left(\underset{\sim}{C}^{e^{-1}}\underline{R}_\sigma + \underset{\sim}{P}_4\underset{\sim}{P}_1^{-1}\underline{R}_\alpha\right) \tag{2.13a}$$

$$\Delta\underline{\alpha}_{n+1}^{k} = -\underset{\sim}{P}_1^{-1}\left(\underline{R}_\alpha - \underset{\sim}{P}_2\Delta\underline{\sigma}_{n+1}^{k}\right) \tag{2.13b}$$

in which J is the iteration Jacobian matrix, and the following definitions are introduced:

$$\underset{\sim}{J} = \underset{\sim}{P}_3 - \underset{\sim}{P}_4\underset{\sim}{P}_1^{-1}\underset{\sim}{P}_2 = \underset{\sim}{C}^{e^{-1}} + \underset{\sim}{P}_4\left(\underset{\sim}{I} - \underset{\sim}{P}_1^{-1}\underset{\sim}{P}_2\right) \tag{2.14a}$$

$$\underset{\sim}{\mathrm{P}}_1 = \underset{\sim}{\mathrm{Z}}_m^{-1} + \underset{\sim}{\mathrm{P}}_2 + \Delta t\gamma\,\underset{\sim}{\mathrm{M}} + \left[\Delta t\gamma' - \frac{\mathrm{h}'}{\mathrm{h}}\left(\Delta t\gamma + 1\right)\right]\underline{\pi}\otimes\underline{\pi} \tag{2.14b}$$

$$\underset{\sim}{P_4} = \Delta t\left(f\,\underset{\sim}{M} + f'\,\underline{\Gamma}\otimes\underline{\Gamma}\right) \quad ; \quad \underset{\sim}{P_2} = h\,\underset{\sim}{P_4} \tag{2.14c}$$

$$\underset{\sim}{P_3} = \underset{\sim}{C^{e^{-1}}} + \Delta t\left(f\,\underset{\sim}{M} + f'\,\underline{\Gamma}\otimes\underline{\Gamma}\right) \tag{2.14d}$$

$$\underline{R_\alpha} = \left(\underset{\sim}{M} - \frac{h'}{h}\,\underline{\pi}\otimes\underline{\pi}\right)\left(\underline{\alpha}_{n+1} - \underline{\alpha}_n\right) - \Delta t\left(hf\,\underline{\Gamma} - \gamma\,\underline{\pi}\right) \tag{2.14e}$$

and the primes indicate "scaled" derivatives as given below (see Eqs. 3.30 in Part I [41]):

$$f' = \frac{1}{k_t^2}\frac{df}{dF} \quad ; \quad h' = \frac{1}{k_t^2}\frac{dh}{dG} \quad ; \quad \gamma' = \frac{1}{k_t^2}\frac{d\gamma}{dG} \tag{2.15}$$

Note that *all* the arrays and functions, e.g. $\underset{\sim}{L}$, $\underline{\Gamma}$, $\underline{\pi}$, f, h etc. in Eqs. (2.13) to (2.14) are evaluated based on the *last* updated state (σ^k_{n+1}, α^k_{n+1}). Note also that the state (σ_n, α_n) corresponds to the *converged* global solution at the last time step; i.e., they are kept *constant* during the local iteration sequence in Eq. (2.12).

2.3. Iterative Solution----Consistent Tangent Stiffness

In keeping with the underlying fully implicit integration scheme, one can straightforwardly proceed to differentiate the updated stress field, σ_{n+1}, to obtain the viscoplastic-moduli or material tangent stiffness matrix, C^{ev}, for use in the finite element stiffness calculations. The derivations will in fact lead to

$$\underset{\sim}{C^{ev}} = \partial\underline{\sigma}_{n+1}/\partial\Delta\underline{\varepsilon} \quad ; \quad d\underline{\sigma} = \underset{\sim}{C^{ev}}\,d\underline{\varepsilon} \tag{2.16a}$$

$$\underset{\sim}{C^{ev}} = \underset{\sim}{J^{-1}} = \left[\underset{\sim}{C^{e^{-1}}} + \underset{\sim}{P_4} - h\,\underset{\sim}{P_4}\,\underset{\sim}{P_1^{-1}}\,\underset{\sim}{P_4}\right]^{-1} \tag{2.16b}$$

Clearly, C^e and $\underset{\sim}{P_1}$, $\underset{\sim}{P_2}$, $\underset{\sim}{P_3}$, $\underset{\sim}{P_4}$ (see Eq. 2.14) are symmetric.

3. Implicit Integration Scheme: NAV Class

In this section, Freed's viscoplastic model [13] is used as an example to discuss the implementation scheme of NAV. The discussion here is limited to the case of an isotropic material under isothermal conditions. A flowchart of the integration scheme is also included in this section.

3.1 General Form

The general form of the integration algorithm described in section 2 may also be used for a nonassociative model. Here the framework of section 2 is utilized to recast the equations of NAV, (given in Part I [41]) and develop the following numerical algorithm. Assume linear hyperelastic response of the model, the Cauchy (true) stress components $\underline{\sigma}$ are given by

$$\underline{\sigma} = \underset{\sim}{C}^{e}\left(\underline{\varepsilon} - \underline{\varepsilon}^{p}\right) \quad ; \quad \underline{\varepsilon} = \underline{\varepsilon}^{e} + \underline{\varepsilon}^{p} \tag{3.1}$$

and $\underset{\sim}{C}^{e}$ is the elastic material matrix. According to eqs. (3.42, 3.47 and 3.49) in Part I [41], the governing equations for NAV are

$$\dot{\underline{\varepsilon}}^{p} = f(J,D)\underline{\Gamma} \quad ; \quad \underline{\Gamma} = \underset{\sim}{M}(\underline{\sigma} - \underline{\alpha}) \tag{3.2}$$

$$\dot{\underline{\alpha}}_{s} = 2\underset{\sim}{Z}\left(H_{s} f \underline{\Gamma} - g_{s}\underline{\pi}_{s}\right) \quad ; \quad \underline{\pi}_{s} = \underset{\sim}{M}\,\underline{\alpha}_{s} \tag{3.3a}$$

$$\dot{\underline{\alpha}}_{l} = 2\underset{\sim}{Z}\left(H_{l} f \underline{\Gamma} - g_{l}\underline{\pi}_{l}\right) \quad ; \quad \underline{\pi}_{l} = \underset{\sim}{M}\,\underline{\alpha}_{l} \tag{3.3b}$$

$$\dot{D} = q_{J} - q_{D} \tag{3.4}$$

where the material functions f, g_s, g_l, q_J, q_D are defined as follows,

$$f = \vartheta A \frac{1}{2\sqrt{J}} Sinh^{n}\left(\frac{\sqrt{J}}{D}\right) \tag{3.5a}$$

$$g_{s} = \frac{H_{s}}{2L_{s}} \vartheta A Sinh^{n}\left(\frac{\sqrt{J}}{D}\right) \tag{3.5b}$$

$$g_I = \frac{H_I}{2L_I}\vartheta A Sinh^n\left(\frac{\sqrt{J}}{D}\right) \tag{3.5c}$$

$$q_J = h_D\left[\frac{\frac{D-D_0}{\delta C}}{Sinh\left(\frac{D-D_0}{\delta C}\right)}\right]^m \vartheta A Sinh^n\left(\frac{\sqrt{J}}{D}\right) \tag{3.5d}$$

$$q_D = h_D\vartheta A\left(\frac{D-D_0}{\delta C}\right)^m Sinh^{(n-m)}\left(\frac{D-D_0}{\delta C}\right) \tag{3.5e}$$

$$J = \frac{1}{2}(\underline{\sigma}-\underline{\alpha})^T \underset{\sim}{M}(\underline{\sigma}-\underline{\alpha}) \tag{3.5f}$$

Note that ϑ, A, H_s, H_I, m, n, D_0, C and δ are material constants, and h_D is a function of the drag stress D (see eq. 3.53 in Part I [41]). Note also that due to the assumption of an isotropic material, ξ, ζ found in the expression for $\underset{\sim}{M}$, (eq. 2.5) are set to zero, thus, $\underset{\sim}{M} = \underset{\sim}{P}$. In this simpler case, following a similar procedure as in section 2, we form the matrix $\underset{\sim}{Z}$, termed the generalized inverse of the deviatoric projection P, for different spaces; e.g., in three-dimensions, we have

$$\underset{\sim}{Z} = \left(\underset{\sim}{P} + \frac{1}{3}\underline{\delta}\otimes\underline{\delta}\right)^{-1} = diag\left[1,1,1,\frac{1}{2},\frac{1}{2},\frac{1}{2}\right] \tag{3.6a}$$

where diag [.] indicates a diagonal matrix with entries in [.]. Also, for generalized plane stress (plates/shells), we have:

$$\underset{\sim}{Z} = \overline{\underset{\sim}{P}}^{-1} \quad ; \quad \overline{\underset{\sim}{P}} = (5\times 5) \ \text{(from } \underset{\sim}{P} \text{ in eq. (3.24a) in Part I [41])} \tag{3.6b}$$

Again, the objective in solving the incremental problem is to find $\sigma_{n+1}, \alpha_{n+1}$ and D_{n+1} at time t_{n+1} based upon the converged values, σ_n, α_n, D_n and $\Delta\varepsilon_n$ at time t_n for the given Δt and $\underline{\Delta\varepsilon}$ whereas n is the step counter. From the rate form of, $\underline{\dot{\sigma}}$, eq. (3.1), the evolution equations (3.2-3.4) $\underline{\dot{\alpha}_s}$, $\underline{\dot{\alpha}_I}$ and $\dot{D}$, and by using the implicit Euler scheme, the following expressions are derived,

$$\underline{\sigma}_{n+1} = \underline{\sigma}_n + \underset{\sim}{C}^e \Delta\underline{\varepsilon} - \Delta t f \underline{\Gamma}_{n+1} \tag{3.7}$$

$$\underline{\alpha_s}_{n+1} = \underline{\alpha_s}_n + 2\Delta t \underset{\sim}{Z}\left(H_s f \underline{\Gamma}_{n+1} - g_s \underline{\pi_s}_{n+1}\right) \tag{3.8a}$$

$$\underline{\alpha_l}_{n+1} = \underline{\alpha_l}_n + 2\Delta t \underset{\sim}{Z}\left(H_l f \underline{\Gamma}_{n+1} - g_l \underline{\pi_l}_{n+1}\right) \tag{3.8b}$$

$$D_{n+1} = D_n + \Delta t(q_J - q_D) \tag{3.9}$$

For a local Newton-Raphson scheme to update state variables, it is necessary to form residual vectors in terms of the variables, i.e.,

$$\underline{R}_\sigma = \underline{\sigma}_{n+1} - \underline{\sigma}_n - \underset{\sim}{C}^e \Delta\underline{\varepsilon} + \Delta t f \underline{\Gamma}_{n+1} \tag{3.10}$$

$$\underline{R}_{\alpha_s} = \underline{\alpha_s}_{n+1} - \underline{\alpha_s}_n - 2\Delta t H_s f \underset{\sim}{Z}\underline{\Gamma}_{n+1} + 2\Delta t g_s \underset{\sim}{Z}\underline{\pi_s}_{n+1} \tag{3.11a}$$

$$\underline{R}_{\alpha_l} = \underline{\alpha_l}_{n+1} - \underline{\alpha_l}_n - 2\Delta t H_l f \underset{\sim}{Z}\underline{\Gamma}_{n+1} + 2\Delta t g_l \underset{\sim}{Z}\underline{\pi_l}_{n+1} \tag{3.11b}$$

$$\underline{R}_\alpha = \underline{R}_{\alpha_s} + \underline{R}_{\alpha_l} \tag{3.11c}$$

$$R_D = D_{n+1} - D_n - \Delta t(q_J - q_D) \tag{3.12}$$

The local iterative update expressions are based on a truncated Taylor's expansion for the $\underline{R}$ vectors about the last updated state, at a typical iteration k $\rightarrow$ k+1

$$\underline{\sigma}^{k+1}_{n+1} = \underline{\sigma}^{k}_{n+1} + \Delta\underline{\sigma}^{k}_{n+1} \tag{3.13}$$

$$\underline{\alpha_s}^{k+1}_{n+1} = \underline{\alpha_s}^{k}_{n+1} + \Delta\underline{\alpha_s}^{k}_{n+1} \tag{3.14a}$$

$$\underline{\alpha_l}^{k+1}_{n+1} = \underline{\alpha_l}^{k}_{n+1} + \Delta\underline{\alpha_l}^{k}_{n+1} \tag{3.14b}$$

$$\underline{\alpha}^{k+1}_{n+1} = \underline{\alpha_s}^{k+1}_{n+1} + \underline{\alpha_l}^{k+1}_{n+1} \tag{3.14c}$$

$$D^{k+1}_{n+1} = D^{k}_{n+1} + \Delta D^{k}_{n+1} \tag{3.15}$$

where expressions for the various increments shown above are as follows:

$$\Delta\underline{\sigma}^{k}_{n+1} = -\underset{\sim}{K}^{-1}\left(\underline{RAB} - \underset{\sim}{PB}\cdot\underset{\sim}{PC}^{-1}\cdot\underline{RDC}\right) \tag{3.16}$$

$$\underline{\Delta\alpha_s}^{k}_{n+1} = -\underset{\sim}{PC}^{-1}\left(\underline{RDC} + \underset{\sim}{PD}\cdot\underline{\Delta\sigma}^{k}_{n+1}\right) \tag{3.17a}$$

$$\underline{\Delta\alpha_l}^{k}_{n+1} = -\underset{\sim}{P_{7l}}^{-1}\left[\underline{R_{\alpha_l}} - \underline{v_{\alpha_l}} + \left(-\underset{\sim}{P_{2l}} + \underset{\sim}{P_{3l}} + \underset{\sim}{P_{6l}}\right)\underline{\Delta\sigma}^{k}_{n+1} + \left(\underset{\sim}{P_{2l}} - \underset{\sim}{P_{3l}} - \underset{\sim}{P_{6l}}\right)\underline{\Delta\alpha_s}^{k}_{n+1}\right] \tag{3.17b}$$

$$\Delta D^{k}_{n+1} = s_9\left(R_D - s_5\underline{\Gamma}\cdot\underline{\Delta\sigma}^{k}_{n+1} + s_5\underline{\Gamma}\cdot\underline{\Delta\alpha_s}^{k}_{n+1} + s_5\underline{\Gamma}\cdot\underline{\Delta\alpha_l}^{k}_{n+1}\right) \tag{3.18}$$

In the above, the scalar quantities, s_1-s_9, relative to the differentials of the material functions in eqs. (3.5), are given as

$$s_1 = \Delta t\, f_D' \quad s_{2s} = 2\Delta t\, H_s f_D' \quad s_{2l} = 2\Delta t\, H_l f_D' \tag{3.19a}$$

$$s_3 = 2\Delta t\, g_{sD}' \quad s_4 = 2\Delta t\, g_{lD}' \quad s_5 = \Delta t\, q_{JJ}' \quad s_6 = 0 \tag{3.19b}$$

$$s_7 = \Delta t\, q_{JD}' \quad s_8 = \Delta t\, q_{DD}' \quad s_9 = \frac{-1}{1 - s_7 - s_8} \tag{3.19c}$$

Where, the second subscript in the primed quantities indicates the variable with respect to which the differentiation is performed. The vectors used in eqs (3.16, 3.17 and 3.18) are relative to the residual function of state variables and are defined as:

$$\underline{v_\sigma} = s_1 s_9 R_D\, \underset{\sim}{C^e}\,\underline{\Gamma} \tag{3.20a}$$

$$\underline{v_{\alpha_s}} = s_9 R_D\left(s_{2s}\,\underset{\sim}{Z}\,\underline{\Gamma} - s_3\,\underset{\sim}{Z}\,\underline{\pi_s}\right) \tag{3.20b}$$

$$\underline{v_{\alpha_l}} = s_9 R_D\left(s_{2l}\,\underset{\sim}{Z}\,\underline{\Gamma} - s_4\,\underset{\sim}{Z}\,\underline{\pi_l}\right) \qquad \underline{v_\alpha} = \underline{v_{\alpha_s}} + \underline{v_{\alpha_l}} \tag{3.20c}$$

$$\underline{RAB} = \underline{R_\sigma} + \underline{v_\sigma} + \left(\underset{\sim}{P_1} - \underset{\sim}{P_5}\right)\underset{\sim}{P_{7l}}^{-1}\left(\underline{R_{\alpha_l}} - \underline{v_{\alpha_l}}\right) \tag{3.21a}$$

$$\underline{RDC} = \underline{R_{\alpha_s}} - \underline{V_{\alpha_s}} - \left(\underset{\sim}{P_{2s}} - \underset{\sim}{P_{3s}} - \underset{\sim}{P_{6s}}\right)\underset{\sim}{P_{7l}}^{-1}\left(\underline{R_{\alpha_l}} - \underline{V_{\alpha_l}}\right) \tag{3.21b}$$

Among the matrices defined in eqs. (3.16, 3.17 and 3.18), $\underset{\sim}{K}$ is the iterative Jacobi matrix, and is defined as

$$\underset{\sim}{K} = \underset{\sim}{PA} - \underset{\sim}{PB}\cdot\underset{\sim}{PC}^{-1}\cdot\underset{\sim}{PD} \tag{3.22}$$

where,

$$\underset{\sim}{PA} = \underset{\sim}{I} + \underset{\sim}{P_1} - \underset{\sim}{P_5} - \left(\underset{\sim}{P_1} - \underset{\sim}{P_5}\right)\underset{\sim}{P_{7l}}^{-1}\left(\underset{\sim}{P_{2l}} - \underset{\sim}{P_{3l}} - \underset{\sim}{P_{6l}}\right) \qquad \underset{\sim}{PB} = \underset{\sim}{I} - \underset{\sim}{PA} \tag{3.23a}$$

$$\underset{\sim}{PC} = \underset{\sim}{P_{7s}} - \left(\underset{\sim}{P_{2s}} - \underset{\sim}{P_{3s}} - \underset{\sim}{P_{6s}}\right)\underset{\sim}{P_{7l}}^{-1}\left(\underset{\sim}{P_{2l}} - \underset{\sim}{P_{3l}} - \underset{\sim}{P_{6l}}\right) \qquad \underset{\sim}{PD} = \underset{\sim}{I} + \underset{\sim}{P_{4s}} - \underset{\sim}{PC} \tag{3.23b}$$

in which matrices $\underset{\sim}{P_1}$ - $\underset{\sim}{P_7}$ result from state variables and their differentials, they are defined as

$$\underset{\sim}{P_1} = \Delta t\, \underset{\sim}{C^e}\left(f\, \underset{\sim}{M} + f_J^{'}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma}\right) \tag{3.24a}$$

$$\underset{\sim}{P_{2s}} = 2\Delta t\, H_s\, \underset{\sim}{Z}\left(f\, \underset{\sim}{M} + f_J^{'}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma}\right) \tag{3.24b}$$

$$\underset{\sim}{P_{2l}} = 2\Delta t\, H_l\, \underset{\sim}{Z}\left(f\, \underset{\sim}{M} + f_J^{'}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma}\right) \tag{3.24c}$$

$$\underset{\sim}{P_{3s}} = 2\Delta t\, \underset{\sim}{Z}\left(g_{sJ}^{'}\, \underset{\sim}{\pi_s} \otimes \underset{\sim}{\Gamma}\right) \qquad \underset{\sim}{P_{3l}} = 2\Delta t\, \underset{\sim}{Z}\left(g_{lJ}^{'}\, \underset{\sim}{\pi_l} \otimes \underset{\sim}{\Gamma}\right) \tag{3.24d}$$

$$\underset{\sim}{P_{4s}} = 2\Delta t\, g_s\, \underset{\sim}{Z}\, \underset{\sim}{M} \qquad \underset{\sim}{P_{4l}} = 2\Delta t\, g_l\, \underset{\sim}{Z}\, \underset{\sim}{M} \tag{3.24e}$$

$$\underset{\sim}{P_5} = s_1 s_5 s_9\, \underset{\sim}{C^e}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma} \tag{3.24f}$$

$$\underset{\sim}{P_{6s}} = s_5 s_9\left(s_{2s}\, \underset{\sim}{Z}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma} - s_3\, \underset{\sim}{Z}\, \underset{\sim}{\pi_s} \otimes \underset{\sim}{\Gamma}\right) \qquad \underset{\sim}{P_{6l}} = s_5 s_9\left(s_{2l}\, \underset{\sim}{Z}\, \underset{\sim}{\Gamma} \otimes \underset{\sim}{\Gamma} - s_4\, \underset{\sim}{Z}\, \underset{\sim}{\pi_l} \otimes \underset{\sim}{\Gamma}\right) \tag{3.24g}$$

$$\underset{\sim}{P_{7s}} = \underset{\sim}{I} + \underset{\sim}{P_{2s}} + \underset{\sim}{P_{4s}} - \underset{\sim}{P_{3s}} - \underset{\sim}{P_{6s}} \qquad \underset{\sim}{P_{7l}} = \underset{\sim}{I} + \underset{\sim}{P_{2l}} + \underset{\sim}{P_{4l}} - \underset{\sim}{P_{3l}} - \underset{\sim}{P_{6l}} \tag{3.24h}$$

Note that all the arrays and functions in eqs. (3.16-3.24) are evaluated based on the last updated state ($\underset{\sim}{\sigma}^{k}_{n+1}$, $\underset{\sim}{\alpha_s}^{k}_{n+1}$, $\underset{\sim}{\alpha_l}^{k}_{n+1}$ and D^{k}_{n+1}) which indicate implicit integration scheme. Finally, the consistent tangent stiffness may be derived directly from integration shceme and is defined as

$$\underset{\sim}{C^{ev}} = \underset{\sim}{K}^{-1}\, \underset{\sim}{C^e} \tag{3.25}$$

Note that $\underset{\sim}{K}$ (defined in eq. 3.22) is no longer symmetric, thus leading to unsymmetric C^{cv}, which is a major difference between the NAV and GVIPS (whose consistent tangent stiffness derived in section 2.3 is symmetric), with significant implication regarding the numerical implementation on both the local- and global- stiffness levels.

3.2 Integration Scheme

As shown above, GVIPS and NAV have the same implementation format, thus, NAV was chosen as the example for presenting the details of the algorithm. The flowchart is included in Appendix I. The box labeled Global Iteration represents the calculation of the structural stiffness and residual force at the global level. The global structural stiffness is based on the current local material stiffnesses that vary with the level of inelasticity involved. The purpose of the material model is to integrate the rate form equations (flow and evolution laws) of the viscoplastic model over the step size Δt and obtain the current material stiffness required for the update of the structural stiffness and the increment of stress $\Delta\sigma$ at the material level. In the flowchart of Appendix I, the subroutines with the m13 prefix are those necessary to perform the implicit integration of NAV. The main subroutine, m13nr5, is a driver subroutine for the implementation of NAV. It calculates increments of stress and internal variables, updates them and checks convergence. Finally, it passes the viscoplastic stiffness matrix, and, converged stress to the global level calculation. Eqs. (3.13-3.21, 3.25) are involved in this subroutine. Subroutine m13heav5 calculates the pretinent material scalar functions (eq. 3.5) and their differentials. Subroutine m13err deals with calculation of the residual functions of stress and internal variables during the local iterations. Eqs. (3.10-3.12) are involved in this subroutine. Subroutine m13k calculates iteration Jacobi matrices of stress and internal variables. Eqs. (3.22-3.24) are implemented in this subroutine. Subroutine m13lines performs line search algorithm discussed in section 4. Other subroutines used in m13nr5 are also introduced in Appendix I.

4 Implementation of Line Search

4.1 Introduction

Although the implicit scheme described above is unconditionally stable, its successful application still requires proper selection of the size of the steps utilized. In this regard two factors are important: (i) accuracy; and (ii) convergence of the local iterations. A simple time-subincrementing strategy was found to be effective in obtaining accurate results especially when dealing with regions of discontinuity in the state space. However, this was found to be insufficient to obtain a computationally efficient solution for a highly nonlinear problem, such as viscoplasticity. When a large time-step size is chosen, too many subincrements are needed, which leads to inefficiency. Thus a more sophisticated solution procedure, namely, a line search algorithm, is required to produce an effective, robust solution algorithm.

The line search technique is an important feature of most numerical techniques for unconstrained optimization and can be used with a wide range of iterative solution procedures such as full Newton-Raphson iteration. It's well known that classical Newton-Raphson is fast and stable only when the trial solution is close to the converged value. For nonlinear problems, the trial solution is usually far away from the real solution, thus full step size of iterative increment vector may cause either wrong direction or out-of-range updated value. The purpose of the line search algorithm is to guide the solution towards convergence, especially when convergence becomes more and more difficult, e.g. using excessive number of iterations, oscillations in residuals, stresses, and displacement norms, and searches for a scalar multiplier that adjusts the amount of the iterative increment vector to be updated within each iteration.

Line search methods were utilized to solve complex nonlinear problems by many researchers. Crisfield [10, 11] applied it to arc-length algorithms to solve concrete cracking problems. In elasto-plastic analyses, Simo and Taylor [43] suggest that the line searches be incorporated with a consistent tangent stiffness. In [43], Simo claims that the use of line search is essential for robust performance of Newton's method. Caddemi and Martin [6] have also demonstrated that in elasto-plastic analysis convergence is not guaranteed unless line search is used.

Among all of the research work mentioned above, the line search method was used to optimize the system of the global equations and minimize the out-of-balance force. Actually, the concept of line search may be applied at either the global (structural) iteration level or at the local (constitutive) iteration level. At the global (structural) level, the concept of the line search algorithm pertains to minimizing the total potential energy, that is, the work done by the residual force due to the iterative displacement. On the local (constitutive) level, it adjusts the suitable increment step of stress and internal variables to guarantee the convergence of the stress and internal variables at material points, and does not involve global iteration. In this report, the line search algorithm was applied to the local level.

4.2 Line Search Strategy

The objective of the line search is to optimize the solution system and minimize the out-of-balance entropy. Thus, a criterion is needed to judge whether or not a given iterative solution is better than a previous one. This criterion takes the form of an objective function or cost function. In the following, some basic concepts are described that are applicable to unconstrained numerical optimization methods.

Instead of using classical Newton iteration scheme in eq. (1.1), the following iterative procedure was utilized:

$$\underline{\Sigma}^{k+1} = \underline{\Sigma}^{k} + \eta \Delta \underline{\Sigma}^{k} \qquad k=0,1,2..... \qquad (4.1)$$

In this equation, the superscript k represents the iteration number, Σ^0 is any starting value, and $\Delta\Sigma^k$ represents an increment value. The iterative scheme described in eq.(4.1) is continued until optimality conditions are satisfied, or an acceptable new value is obtained. Here, Σ^k represents the state variable vector associated with a viscoplastic constitutive model algorithm. For the GVIPS model,

$$\Sigma^k = \begin{pmatrix} \underline{\sigma}^k \\ \underline{\alpha}^k \end{pmatrix} \tag{4.2a}$$

and for the NAV model,

$$\Sigma^k = \begin{pmatrix} \underline{\sigma}^k \\ \underline{\alpha_s}^k \\ \underline{\alpha_l}^k \\ \underline{D}^k \end{pmatrix} \tag{4.2b}$$

Define a scalar function f as the objective function to be optimized as follows:

$$f(\underline{\Sigma}) = \int \underline{R} \cdot d\underline{\Sigma} \quad ; \quad df = \underline{R} \cdot d\underline{\Sigma} \tag{4.3}$$

where, $\underline{R}$ is the residual function of the state variables. Symbol "." indicates dot product of two vectors. Again for the GVIPS model,

$$\underline{R}^k = \begin{pmatrix} \underline{R}_\sigma^k \\ \underline{R}_\alpha^k \end{pmatrix} \tag{4.4a}$$

and for the NAV model,

$$\underline{R}^k = \begin{pmatrix} \underline{R}_\sigma^k \\ \underline{R}_{\alpha_s}^k \\ \underline{R}_{\alpha_l}^k \\ R_D^k \end{pmatrix} \tag{4.4b}$$

For unconstrained problems, the residual comes from the difference between the current value and the previous converged value. The calculations for $\Delta\underline{\Sigma}$ depend on the residual function and its derivatives at the previous step. In order to reach a minimum point for the objective function $f(\underline{\Sigma})$, a suitable value of the scalar η must be found, such that

$$f(\underline{\Sigma}^{k+1}) = f(\underline{\Sigma}^{k} + \eta\Delta\underline{\Sigma}^{k}) \tag{4.5}$$

is a minimum.

Assume $\Delta\underline{\Sigma}^{k}$ is known at iteration k. According to the stationary condition:

$$\frac{df(\underline{\Sigma}^{k+1})}{d\eta} = \frac{\partial f(\underline{\Sigma}^{k+1})}{\partial \underline{\Sigma}} \cdot \frac{d\underline{\Sigma}^{k+1}}{d\eta} = \frac{\partial f(\underline{\Sigma}^{k+1})}{\partial \underline{\Sigma}} \cdot \Delta\underline{\Sigma}^{k} = 0 \tag{4.6}$$

From eq. (4.3), eq(4.6) becomes:

$$\underline{R}^{k+1} \cdot \Delta\underline{\Sigma}^{k} = 0 \tag{4.7}$$

Now consider,

$$s(\eta) = \underline{R}(\eta) \cdot \Delta\underline{\Sigma}^{k} \tag{4.8}$$

in which $\underline{\Sigma}^{k}$ and $\Delta\underline{\Sigma}^{k}$ are fixed, and $\underline{R}$ and s are functions of η. When $\eta = 0$,

$$s_0 = s(\eta=0) = \Delta\underline{\Sigma}^{k} \cdot \underline{R}(\eta=0) = \Delta\underline{\Sigma}^{k} \cdot \underline{R}_0 \tag{4.9}$$

$\underline{R}_0$ is the residual function of stress and the internal variables at the end of the previous iteration. According to optimization theory, the best (optimum) solution is $s(\eta) = 0$, but numerically, this is not realistically possible and it is inefficient to try and achieve this objective. In practice, a 'slack' line search is used, see Fig 1, wherein the objective is to make the modulus of $s(\eta)$ small in comparison to the modulus of s_0, i.e.

$$|r(\eta)| = \left|\frac{s(\eta)}{s_0}\right| < \beta_{ls} \tag{4.10}$$

where β_{ls} is the 'line-search tolerance'. Based on past research experience, a suitable value for β_{ls} is on the order of 0.8 [11].

4.3 Search for η

In the line search procedure, a key step is the search for an optimum η for which the requirement (eq. (4.8)) is met. Crisfield [11] suggests using a simple linear interpolation and extrapolation. Usually no more than two searches for η are necessary. Initially, $s_0/s_0 = 1$ at $\eta_0=0$, and the line search is started using $\eta=1$, which

corresponds to the basic Newton-Raphson iteration. From eq.(4.8), $s_1 = s(\eta=1)$, thus the initial search for a new "improved" value for η (denoted as η_1 in Fig. 2) completely depends on the value of s_1/s_0 (see point "1" in Fig. 2). Figures (2-3) show four possibilities, but the case most frequently encountered is that shown in fig. 2.

Because of the stiff behavior of the viscoplastic model, $\Delta\underline{\Sigma}$ may be very large especially if a large time-step size is chosen. Consequently, the residual function may also be very large, i.e. $| s_1 |$ may be very large, which leads to a very small η_1 after linear interpolation. Thus, a double interpolation is used by means of s_2/s_0 (denoted as point "2" in Fig. 2) and either s_0/s_0 (Fig. 2a) or s_1/s_0 (Fig. 2b) to obtain an updated value η_2 which is more accurate than η_1. Note that a minimum of 0.01 is set for η.

Consider Figure 3a, which is a possible extrapolation case. When s_1/s_0 is near 1.0, extrapolation could result in a large η which could lead to excessive iterations. Even if η is not very large, as found in the present research a value of η which is less than 1 is used to speed iteration. For example, Crisfield [11] suggests a maximum value of 10.0 for η when considering concrete cracking analysis. In a similar fashion, negative extrapolation of Fig. 3b is not used in the model implementation. Theoretically, this could not happen because of the hardening behavior of viscoplasticity, only a softening problem may behave like this. Thus, if either of the cases described in Figure 3 occur, η is assumed to be 1 which is the regular Newton-Raphson iterative method.

Numerical tests have shown (refer to Part I [41]) that the use of line search leads to significant improvement in the convergence and computational efficiency with regards to CPU time and iterations. It has also been shown that line search helps convergence greatly for the nonassociative viscoplastic model such that subincrements are not required. The only additional computational effort, in comparison with a formulation without line searches, would be the calculation of the inner product (eq. 4.8) which is considered to be almost negligible.

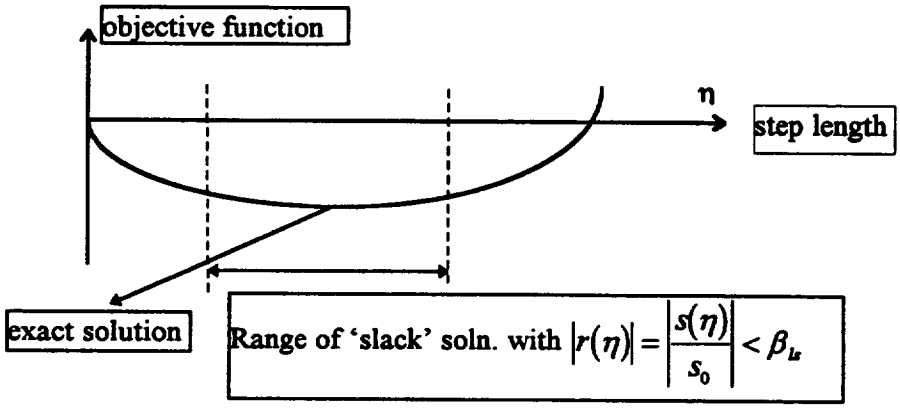

Figure 1 Schematic of line search

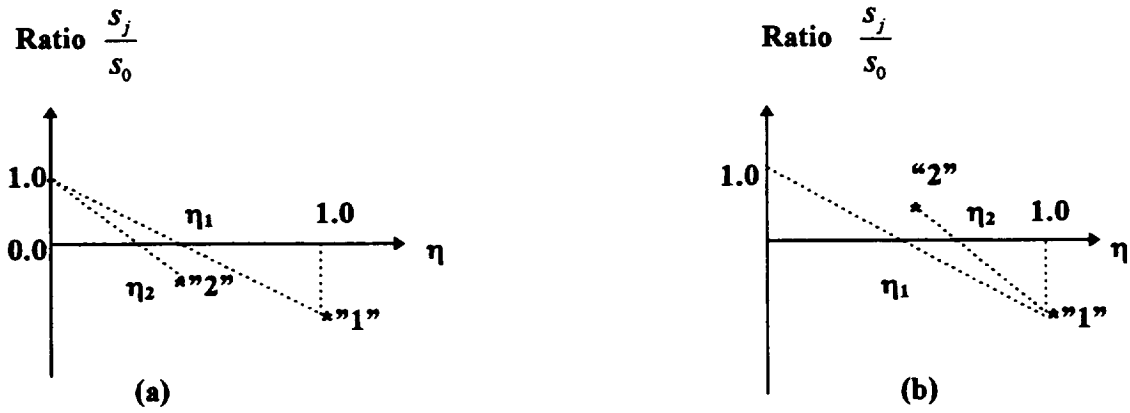

Figure 2 Interpolation Schematic

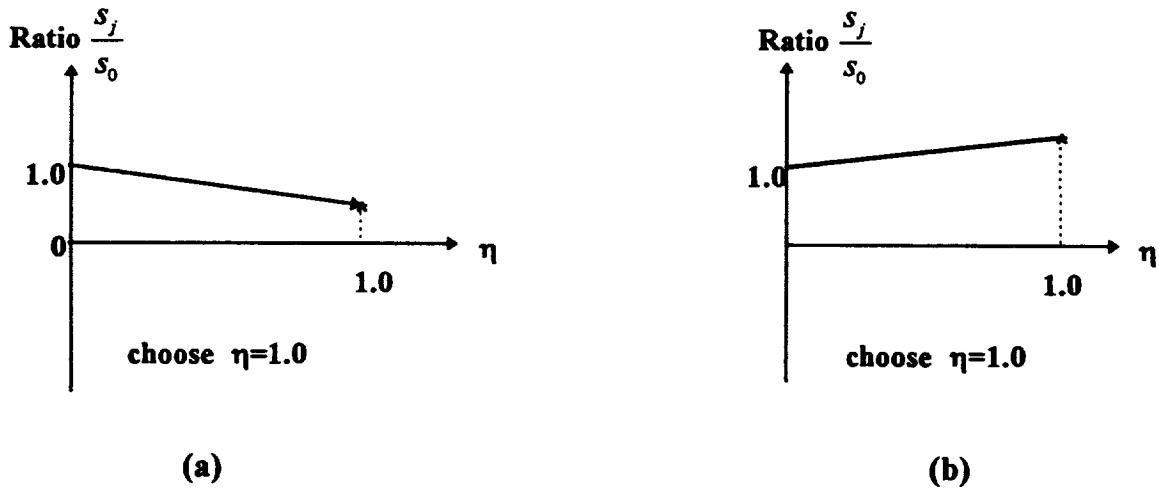

Figure 3 Extrapolation Schematic

5. Summary and Conclusions

The general computational framework using a fully implicit backward Euler integration method has been presented and has been shown [41] to be successful for both the Generalized Viscoplasticity with Potential Structure (GVIPS) and Non-associative Viscoplastic models (NAV). Original equations for the NAV model developed by Freed are recast into a matrix format similar to that used for GVIPS in order to facilitate the model's implementation into the newly developed framework. Only these Newton iterative schemes developed herein will provide, uniformly-valid, convergent, robust integration for both GVIPS and NAV. The algorithm was written in a concise matrix format so as to provide sufficient generality and is automatically valid for both isotropic and anisotropic cases in either full space or subspaces.

The "slack" method, which is the form of line search used in the present algorithm, enables GVIPS and NAV to converge stably, with sufficient accuracy, and significantly improved efficiency. Convergence may be achieved for large load steps, whereas traditional fixed stepping without line search will fail. Thus, the proposed computational framework makes the solution of realistic nonlinear finite element analysis problems possible. The only additional computational effort of line search method in comparison with a formulation without line search, would be the calculation of the inner product, which is believed to be negligible as compared to the total calculations involved in a nonlinear finite element analysis.

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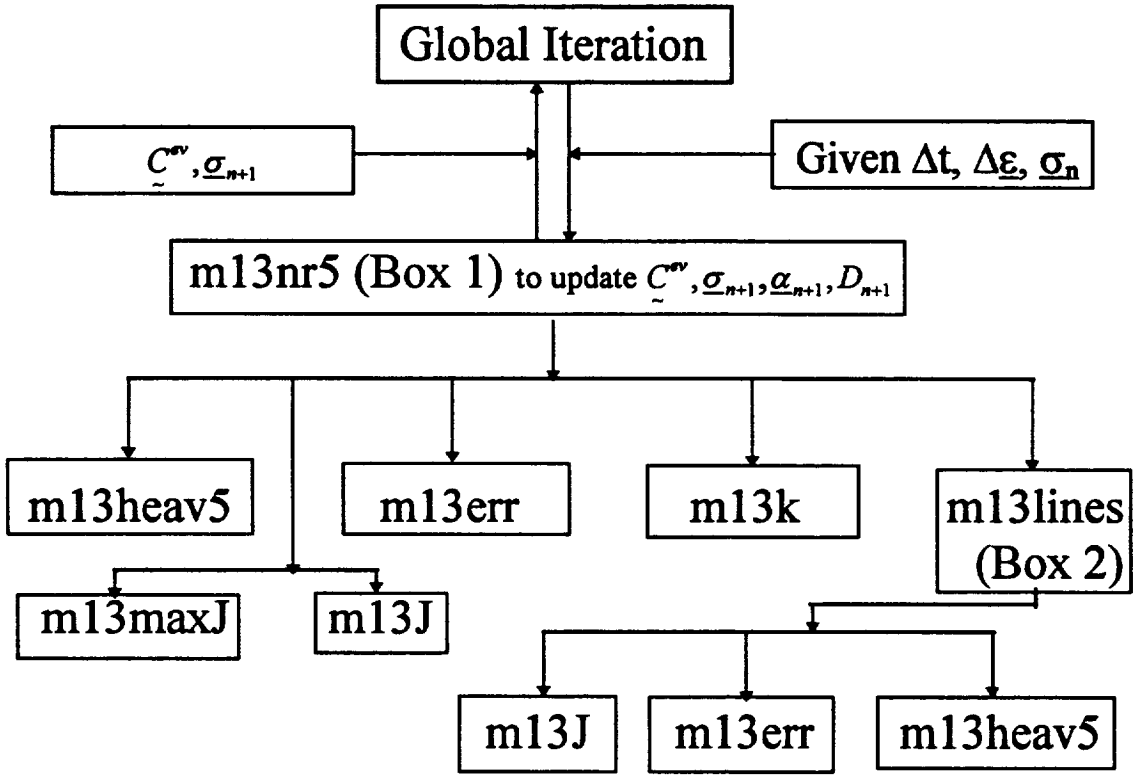
Appendix I: Flowchart for Implicit Integration Algorithm



m13nr5------- Driver for performing implicit integration of rate-dependent equations
m13heav5---- Calculate step or smoothing functions
m13err------- Calculate error functions during local iteration
m13k--------- Calculate Jacobi matrix during local iteration
m13lines------ Perform line search algorithm
m13j---------- Calculate invariance, i.e., eq. (3.6f)
m13maxj------ Calculate maximum invariance

Box 1

Iterative procedure (subroutine m13nr5)

1. Given $\underline{\sigma}_n, \underline{\alpha}_n^s, \underline{\alpha}_n^l, D_n, \Delta\underline{\varepsilon}, \Delta t$.

   k=0, $\underline{\sigma}_{n+1}^0 = \underline{\sigma}_n ; \underline{\alpha_s}_{n+1}^{\ 0} = \underline{\alpha_s}_n ; \underline{\alpha_l}_{n+1}^{\ 0} = \underline{\alpha_l}_n ; D_{n+1}^0 = D_n$

2. Evaluate material function and differentiation. (subroutine m13heav5)

   f, g, q_J, q_D, f_D, ...

3. Evaluate residual function (subroutine m13err)

   $\underline{R}_\sigma(\underline{\sigma}_{n+1}^k)$, $\underline{R}_{\alpha_s}\left(\underline{\alpha_s}_{n+1}^{\ k}\right)$, $\underline{R}_{\alpha_l}\left(\underline{\alpha_l}_{n+1}^{\ k}\right)$, $R_D\left(D_{n+1}^k\right)$

   $$\underline{R}_{n+1}^k = \left\{\underline{R}_\sigma, \underline{R}_{\alpha_s}, \underline{R}_{\alpha_l}, R_D\right\}^T$$

4. Evaluate Jacobi matrix $\underset{\sim}{K}$ (subroutine m13k)

5. Evaluate $\Delta\underline{\sigma}_{n+1}^k, \Delta\underline{\alpha_s}_{n+1}^{\ k}, \Delta\underline{\alpha_l}_{n+1}^{\ k}, \Delta D^k$

   $$\Delta\underline{\Sigma}_{n+1}^k = \{\ \Delta\underline{\sigma}_{n+1}^k, \Delta\underline{\alpha_s}_{n+1}^{\ k}, \Delta\underline{\alpha_l}_{n+1}^{\ k}, \Delta D^k\ \}^T$$

6. evaluate current value.

   $$\underline{\sigma}_{n+1}^{k+1} = \underline{\sigma}_{n+1}^k + \Delta\underline{\sigma}_{n+1}^k$$
   $$\underline{\alpha_s}_{n+1}^{\ k+1} = \underline{\alpha_s}_{n+1}^{\ k} + \Delta\underline{\alpha_s}_{n+1}^{\ k} \ ; \ \underline{\alpha_l}_{n+1}^{\ k+1} = \underline{\alpha_l}_{n+1}^{\ k} + \Delta\underline{\alpha_l}_{n+1}^{\ k}$$
   $$D_{n+1}^{k+1} = D_{n+1}^k + \Delta D_{n+1}^k$$

7. Evaluate residual function based on current value. (subroutine m13err)

   $\underline{R}_\sigma(\underline{\sigma}_{n+1}^{k+1})$, $\underline{R}_{\alpha_s}\left(\underline{\alpha_s}_{n+1}^{\ k+1}\right)$, $\underline{R}_{\alpha_l}\left(\underline{\alpha_l}_{n+1}^{\ k+1}\right)$, $R_D\left(D_{n+1}^{k+1}\right)$

   $$\underline{R}_{n+1}^{k+1} = \left\{\underline{R}_\sigma, \underline{R}_{\alpha_s}, \underline{R}_{\alpha_l}, R_D\right\}^T$$

Box 1 continued:

8. if $\left|\Delta\underline{\Sigma}^{k}_{n+1} \bullet \underline{R}^{k+1}_{n+1}\right| \geq \left|\Delta\underline{\Sigma}^{k}_{n+1} \bullet \underline{R}^{k}_{n+1}\right|$ then

goto Box 2 (line search algorithm -- subroutine m13lines)

endif

9. Check convergence.

if $\dfrac{\left|\underline{\sigma}^{k+1}_{n+1} - \underline{\sigma}^{k}_{n+1}\right|}{\left|\underline{\sigma}^{k+1}_{n+1}\right|} \geq Tol$ then

k=k+1

goto 2.

else

$\underline{\sigma}_{n+1} = \underline{\sigma}^{k+1}_{n+1}$

$\underline{\alpha_s}_{n+1} = \underline{\alpha_s}^{k+1}_{n+1}$

$\underline{\alpha_l}_{n+1} = \underline{\alpha_l}^{k+1}_{n+1}$

$D_{n+1} = D^{k+1}_{n+1}$

10. Evaluate $\underset{\sim}{K}$ based on converged value and stiffness matrix.

(subroutine m13k)

$\underset{\sim}{C}^{ev} = \underset{\sim}{K}^{-1}\,\underset{\sim}{C}^{e}$

return

end

Box 2.

Line search scheme (subroutine m13lines)

1.Initialize

$\Delta\underline{\Sigma}_{n+1}^{k}, \underline{\Sigma}_{n+1}^{k}, \eta_a = 1, \eta_b = 0, \underline{R_a} = \underline{R}_{n+1}^{k+1}, \underline{R_b} = \underline{R}_{n+1}^{k}$

2. Bracketing

IF $\text{sign}\left(\Delta\underline{\Sigma}_{n+1}^{k} \bullet \underline{R_a}\right) \text{x sign}\left(\Delta\underline{\Sigma}_{n+1}^{k} \bullet \underline{R_b}\right) < 0$ then

interplotating, find η.

evaluate $\underline{\Sigma}_{n+1}^{\eta} = \underline{\Sigma}_{n+1}^{k} + \eta\Delta\underline{\Sigma}_{n+1}^{k}$

evaluate residual function based on $\underline{\Sigma}_{n+1}^{\eta}$ (subroutine m13err)

$\underline{R}_{\sigma}(\underline{\sigma}_{n+1}^{\eta})$, $\underline{R}_{\alpha_s}\left(\underline{\alpha_s}_{n+1}^{\eta}\right)$, $\underline{R}_{\alpha_l}\left(\underline{\alpha_l}_{n+1}^{\eta}\right)$, $R_D\left(D_{n+1}^{\eta}\right)$

$\underline{R_\eta} = \left\{\underline{R_\sigma}, \underline{R_{\alpha_s}}, \underline{R_{\alpha_l}}, R_D\right\}^{\mathrm{T}}$

IF $\text{sign}\left(\Delta\underline{\Sigma}_{n+1}^{k} \bullet \underline{R_\eta}\right) \text{x sign}\left(\Delta\underline{\Sigma}_{n+1}^{k} \bullet \underline{R_b}\right) < 0$ then

interplotaing new η between η_b and η

else

interplotaing new η between η_a and η

endif

ELSE

η=1

ENDIF

IF(η < Min.) η=Min.

3. Update

$\underline{\Sigma}_{n+1}^{k+1} = \underline{\Sigma}_{n+1}^{k} + \eta\Delta\underline{\Sigma}_{n+1}^{k}$

4. Return.

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13. ABSTRACT (*Maximum 200 words*)

This two-part report is concerned with the development of a general framework for the implicit time-stepping integrators for the flow and evolution equations in generalized viscoplastic models. The primary goal is to present a complete theoretical formulation, and to address in detail the algorithmic and numerical analysis aspects involved in its finite element implementation, as well as to critically assess the numerical performance of the developed schemes in a comprehensive set of test cases. On the theoretical side, the general framework is developed on the basis of the unconditionally-stable, backward-Euler difference scheme as a starting point. Its mathematical structure is of sufficient generality to allow a unified treatment of different classes of viscoplastic models with internal variables. In particular, two specific models of this type, which are representative of the present start-of-art in metal viscoplasticity, are considered in applications reported here; i.e., fully associative (GVIPS) and non-associative (NAV) models. The matrix forms developed for both these models are directly applicable for both initially isotropic and anisotropic materials, in general (three-dimensional) situations as well as subspace applications (i.e., plane stress/strain, axisymmetric, generalized plane stress in shells). On the computational side, issues related to efficiency and robustness are emphasized in developing the (local) interative algorithm. In particular, closed-form expressions for residual vectors and (consistent) material tangent stiffness arrays are given explicitly for both GVIPS and NAV models, with their maximum sizes "optimized" to depend only on the number of independent stress components (but independent of the number of viscoplastic internal state parameters). Significant robustness of the local iterative solution is provided by complementing the basic Newton-Raphson scheme with a line-search strategy for convergence. In the present second part of the report, we focus on the specific details of the numerical schemes, and associated computer algorithms, for the finite-element implementation of GVIPS and NAV models.

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